3DVC_Red3_MinimumRequirements

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What are Minimum requirements for a 3D virutal cell?

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What are the minimum requirements to make something useful/reusable

Software components and public API to build a model

What is a model (in the sense of simulation)?

Cell simulation of microplasma (one second intervals) – minimum requirements “we have simulated a cell” => Getting this for a human cell

No information where one protein is, but higher order interactions

What is our goal?
Do you simulate one cell cycle?
Do you provide a fly-through?

The 3D virtual cell is more than just one model, but it is a useful umbrella for many different types of models. This is a young field, the paradigms are few. Some established types of models are
Interaction diffusion model
Transcriptional networks
Metabolic networks
Putting together the different approaches is making the idea of this community most interesting. Each of the models needs experimental data as input, needs to verify the models.

Define a set of components, and how they interact.

Define cell behaviors without using model assumptions (they grow, divide, stick to each other, etc.)

We need ontologies describing the components and standards for the components to interact.

We need a registry to register components
We need tools / software / to do something with the components.
How can I find tools that help me to do something?
We need libraries to build tools.

Should NIH come on board to help fund the infrastructure? NSF has the research grants? There is examples from data visualisation.

in cell based models you have many models. you are logical, rather than mathematical. describe biologically what each cell does. How this is translated into code, who knows. There are frameworks for rule based models (they are horrible) . These frameworks can lead to conclusions. Some critical comments about that.

Are there other type of models? “relational grounding” CS has come up with concepts that are valuable for modeling. Programming languages have been designed for that. Idea that models can be described independent from their implementation.

There are cases where the code is the model

You need some language to express some models.